3-D Inorganic Crystal Structure Generation and Property Prediction via Representation Learning

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Abstract

Generative models have been successfully used to synthesize completely novel images, text, music, and speech. As such, they present an exciting opportunity for the design of new materials for functional applications. So far, generative deep-learning methods applied to molecular and drug discovery have yet to produce stable and novel 3-D crystal structures across multiple material classes. To that end, we, herein, present an autoencoder-based generative deep-representation learning pipeline for geometrically optimized 3-D crystal structures that simultaneously predicts the values of eight target properties. The system is highly general, as demonstrated through creation of novel materials from three separate material classes: binary alloys, ternary perovskites, and Heusler compounds. Comparison of these generated structures to those optimized via electronic-structure calculations shows that our generated materials are valid and geometrically optimized.